THE DESIGN OF A QUANTAL RESPONSE EXPERIMENT: AN EMPIRICAL APPROACH

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ABSTRACT
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An important issue in quantal response estimation problems considered by Mazzuchi and Singpurwalla (1982) is the design of the experiment. The objective there was to estimate the probability of response for a given stimulus, but due to the expense of the items, testing has to be kept to a minimum. As a continuation of the work by Mazzuchi and Singpurwalla (1982), we address this problem and present a criterion for comparing several designs that are of interest.

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1. INTRODUCTION

The U.S. Army Kinetic Energy Penetrator problem has been described by Mazzuchi and Singpurwalla (1982), henceforth MS. Their objective was to estimate the relationship between the striking velocity (the stimulus) and the probability of penetration of a projectile. This is a quantal response experiment in which the goal is to estimate the probability of response for a given stimulus.

The strategy used to test the effectiveness of the penetrator is to fix an angle of fire and then to fire the penetrator at different striking velocities. After each firing, the outcome, success or failure, is recorded.

The equipment used in testing is expensive, and thus testing is kept to a minimum. Typically, an experimenter is allowed a fixed number of tests. That is, a fixed number of copies of the penetrator can be tested at different striking velocities. Therefore, designing the experiment in an optimal way is an important issue. In a quantal response

problem, the investigator is also interested in estimating the striking velocity (stimulus), say V_α , at which the probability of penetration (response) is α . Thus, the experiment should be designed in a way that will provide the investigator with a "good" estimate of the V_α , for a specified amount of testing.

In this report, we attempt to present an approach that may be helpful in designing an experiment which addresses the objectives mentioned above. Due to the nature of the penetrator problem, interest generally centers around $V_{.05}$ and $V_{.95}$, stimuli at which the probabilities of response are 0.05 and 0.95 , respectively. In our analysis, we will focus attention on the former.

2. AN OUTLINE OF THE APPROACH

Suppose that the experimenter is allowed to test k copies of the penetrator at k distinct levels of the stimuli. Our goal is to select the k distinct levels of stimulus in a way that will provide us a "good" estimate of $V_{.05}$.

To estimate $V_{.05}$, we first estimate the response curve based on the k distinct firings. The approach discussed in MS is adcpted.

Let $V_1 < V_2 < \cdots < V_k$ be k distinct levels of the stimulus. Since our aim is to select these k distinct levels in an "optimal" way, different designs have to be considered in the analysis. Because actual testing under the various designs is not practically feasible, our analysis is based on a simulation.

2.1 Simulation of the Responses

The outcome of a test at V_i is described by a binary variable X_i , $i = 1,2,\ldots,k$, where $X_i = 1$ if the target is defeated and $X_i = 0$ otherwise. To simulate the outcome X_i of a test at stimulus V_i , we assume that we know the "true" probability of response at V_i , $i = 1,2,\ldots,k$.

Let $V_1 < V_2 < \ldots < V_k$ be the selected levels of stimulus for the experiment; then $(V_1, V_2, \ldots, V_k)$ is the selected design. Let $R(v)$ be the "true" response curve; the response curves considered here are cumulative distribution functions. Thus, the true probability of response p_i at stimulus V_i is $R(V_i)$. Next we generate a random variable, U_i , from a uniform distribution over (0,1) and set $X_i = 1$ if $U_i \leq p_i$, and $X_i = 0$ if $U_i > p_i$. Thus the outcome for a given design is a k-dimensional vector of 0's and 1's.

Once $\underset{\sim}{X} = (X_1, X_2, \ldots, X_k)$ is obtained, the probabilities of response, p_i's , $i = 1,\ldots,k$, can be estimated using the approach discussed in MS.

2.2 Estimation of $V_{.05}$

To estimate the probability of response, p_i , for each V_i , $i = 1,2,\ldots,k$, we assign a Dirichlet as a prior distribution for the successive differences $p_1, p_2-p_1, \ldots, p_k-p_{k-1}$ and the modal value of the joint posterior distribution is a Bayes point estimate of $(p_1,\ldots,p_k)$. The computation of the modal value of the joint posterior distribution necessitates the use of an optimization algorithm; this is described by Mazzuchi and Soyer (1982).

The specification of the prior parameters of the Dirichlet distribution is also discussed in MS.

Once estimates of the p_i's are obtained, an estimate of $V_{.05}$ can be obtained by constructing an estimated response curve. The estimated response curve is a plot of the levels of stimulus V_i, versus the $\hat{p}_i$'s, the estimated probabilities of response, $i = 1,2,\ldots,k$. Once such a plot is obtained, the interpolation procedure described in MS is used to estimate $V_{.05}$.

Specifically, for the estimation of $V_{.05}$, we first see if there is an observed stimulus, V_i, for which $\hat{p}_i = 0.05$. If so, then V_i is the estimate of $V_{.05}$. If not, the pair of observational stimuli, say V_i and V_{i+1}, for which $\hat{p}_i < 0.05 < \hat{p}_{i+1}$, are determined. Since the response curve is increasing, the straight line segment joining the points $0, \hat{p}_1, \ldots, \hat{p}_i, \hat{p}_{i+1}, \ldots, \hat{p}_k, 1$, will be an increasing function of i. We can find the value of the stimulus, say $\hat{V}_{.05}$, $V_i < \hat{V}_{.05} < V_{i+1}$, for which $\hat{p} = 0.05$ (as indicated in Figure 1).

2.3 Comparison of Designs

The goal of our analysis is to select a design, $(V_1,\ldots,V_k)$, which will provide a "good" estimate of $V_{.05}$.

In order to determine an optimal choice of the k distinct levels of stimulus, we consider different designs, and first obtain an estimate of $V_{.05}$ for each design. Let $(V_1^j, \ldots, V_k^j)$ denote design j; the superscript j indicates a particular design. Once a j is chosen, we obtain $\underset{\sim}{X}^j = (X_1^j, \ldots, X_k^j)$ using the approach discussed in

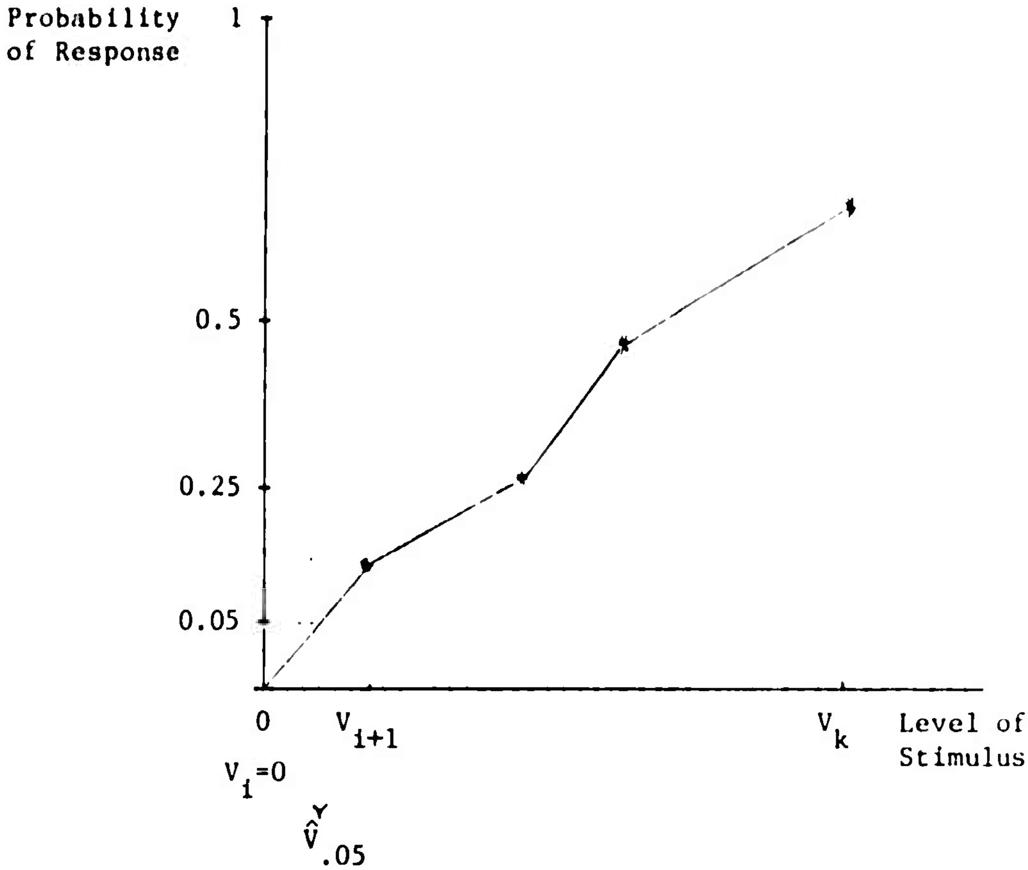

Figure 1. Interpolation procedure.

Section 2.2. Then via the estimated response curve, we obtain an estimate of $V_{.05}$, say $\hat{V}^j_{.05}$. Since the "true" response curve is assumed to be known, the estimate $\hat{V}^j_{.05}$ can be compared with the true value of $V_{.05}$.

If the above procedure is repeated for a different design, a different response curve is estimated. The various estimated response curves provide us with different estimates of $V_{.05}$, and we need to determine which of the designs gives us estimates which are closest to $V_{.05}$. Note that, since the outcome $\underset{\sim}{X}^j = (X^j_1, \ldots, X^j_k)$ for design j is obtained by simulation, different replications of $\underset{\sim}{X}^j$ can be obtained by using different <u>seeds</u> in the simulation.

Let N be the number of replications which are analyzed for design j. For each replication of $\underset{\sim}{X}^j$, a different response curve is estimated and therefore a different estimate of $V_{.05}$, say $\hat{V}^j_{.05}(\ell)$, is obtained. Since we know the true value of $V_{.05}$, the mean squared error (MSE) for design j is computed as

$$MSE^j = \sum_{\ell=1}^{N} (\hat{V}^j_{.05}(\ell) - V_{.05})^2 .$$

The MSE for each design can be obtained and a comparison of the MSE's provides us with a criterion for selecting a good design. The design with the minimum MSE is a good design for a known response curve, say $R_i(v)$. It is possible that a design which is good for $R_i(v)$ may not be good for $R_k(v)$, $i \neq k$. This possibility has also been considered in our analysis.

3. SUMMARY

The approach we presented in Section 2 is applied to some simulated data in the next section.

Three different "true" response curves are selected. These curves are chosen in such a way that they will provide us with different values of $V_{.05}$.

The first response curve is specified via a Weibull distribution function,

$$R_1(v_i) = 1 - \exp\left\{-\left(\frac{v_i}{100}\right)^2\right\}, \text{ where } V_{.05} = 22 .$$

The second is via a lognormal distribution function,

$$R_2(v_i) = \Phi\left(\frac{\log_e v_i - 4.50}{0.33}\right) , \quad \text{where} \quad V_{.05} = 52$$

and Φ denotes the standard normal distribution function.

The third response curve considered is also a lognormal distribution function, which gives $V_{.05} = 10$; that is,

$$R_3(v_i) = \Phi\left(\frac{\log_e v_i - 3.3}{0.6}\right) .$$

Five different designs are selected and analyzed.

Design 1 -- the k observations are distributed evenly over the entire interval of the range of testing, say I .

Design 2 -- all the k observations are concentrated on the left-hand half of I .

Design 3 -- all the k observations are concentrated in the center of I .

Design 4 -- all the k observations are concentrated on the right-hand half of I .

Design 5 -- the k observations are sequentially obtained in three different phases.

The value of k is (arbitrarily) chosen as 12, and due to the expense of simulation, ten different replications of $\underset{\sim}{X}^j$ are considered.

The MSE's for each design based on the ten replications are computed, on the basis of which it is felt that Design 3 is a suitable design for the estimation of $V_{.05}$.

4. APPLICATION TO SOME SIMULATED DATA

The three "true" response curves discussed in Section 3 are analyzed separately in this section. These response curves are illustrated in Figures 2, 3, and 4. A replication, simulated from each of these response curves, is presented in the Appendix for illustration.

We assume that the probability of a response at a striking velocity of 300 is almost 1. Thus we make an arbitrary choice for our best prior guess of p_i, say p_i^*, by letting $p_i^* = 1 - \exp[-0.0307\ V_i]$. The prior parameters are chosen as described in MS. In our analysis the smoothing parameter is chosen as $\beta = 10$.

The five different designs presented in Section 3 will be used in the analysis. In the first four designs, the penetrator is tested in a single phase. In Design 1, the 12 observations are taken equally spaced over the entire range of testing, (0,300). In Design 2 all 12 observations are taken equally spaced on the left-hand half of the interval (0,150). In Designs 3 and 4 the 12 observations are taken equally spaced in the center, and on the right-hand half of the interval, respectively.

The sequential design, Design 5, consists of three phases. In the first phase, six observations are taken equally spaced over the entire range of testing. Ten different replications of the outcome vector, $\underset{\sim}{X}$, are examined and the experimenter tries to identify two regions: one region where the outcome is zero and another where the outcome is one most of the time. Once these two regions are determined, the experimenter has knowledge about the region where the response is

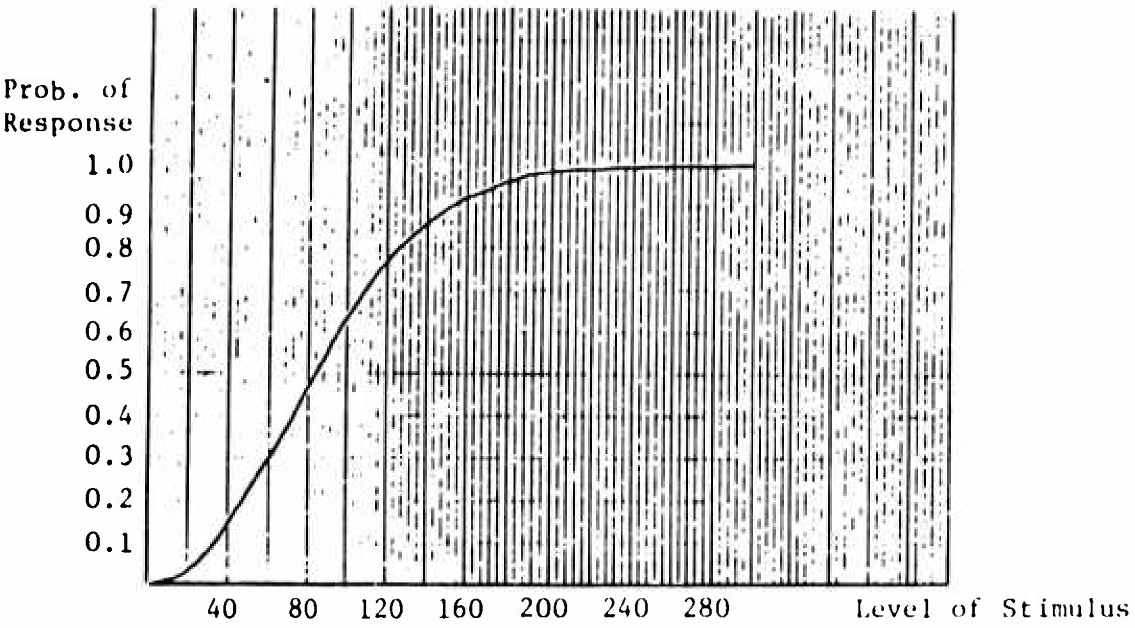

Figure 2. Weibull response curve.

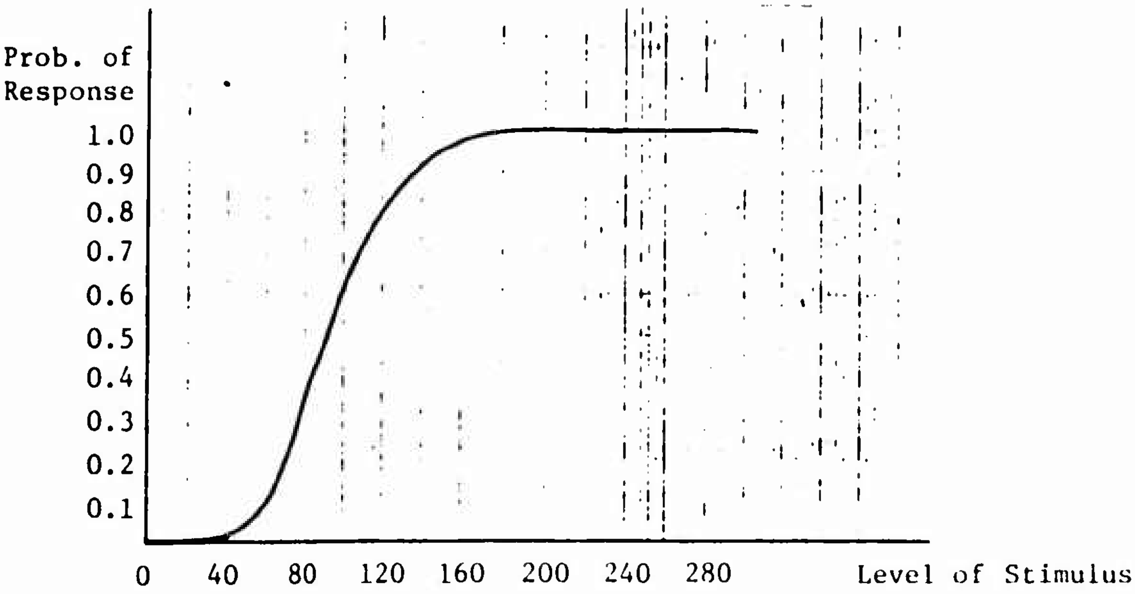

Figure 3. Lognormal response curve I.

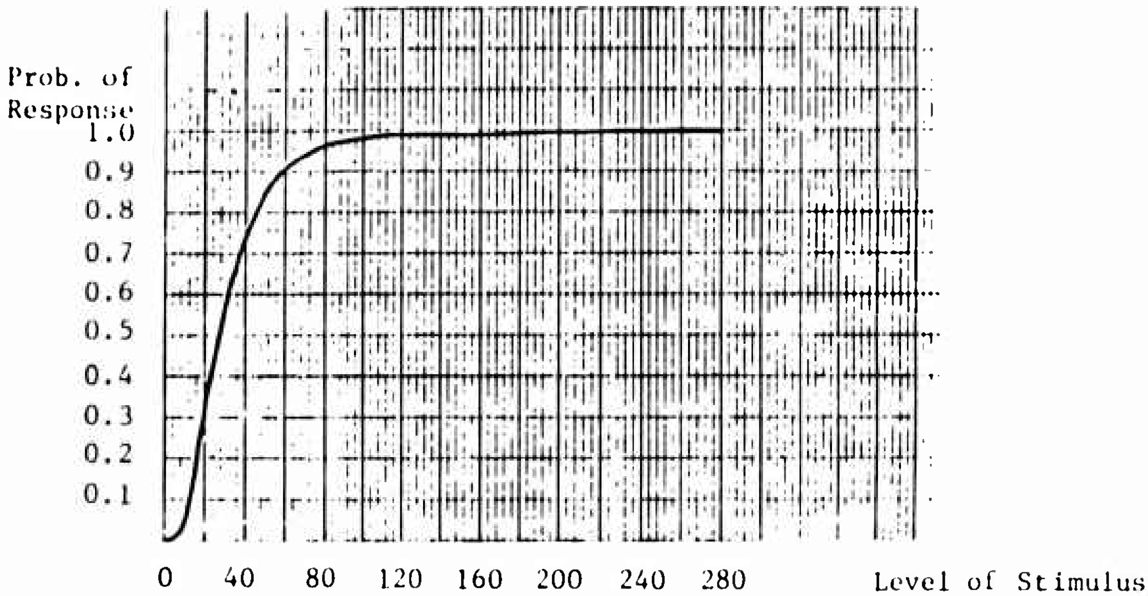

Figure 4. Lognormal response curve II.

most likely to change. In phase 1 of the experiment a new response curve is also estimated, and this curve provides the prior values of p_i's for the second phase. In the second phase, three observations are taken, equally spaced over the region where the response is most likely to change, as is indicated by phase 1 and a new response curve estimated based on these observations and the prior (the posterior from phase 1). In the final phase of the experiment, the remaining three observations are taken on the left-hand end of our best guess based on phase 2 and a new response curve is estimated using these observations and the prior (the posterior from phase 2). The estimate of $V_{.05}$ is obtained by using this updated response curve.

The outcomes of the five different designs are presented in the Appendix, Tables A.1 - A.3.

4.1 Analysis for the Weibull Response Curve

The first response curve that is considered is a Weibull distribution function for which $V_{.05} = 22$. The outcome vector, $\underset{\sim}{X}^j$ for $j = 1,\ldots,4$, is simulated using this response curve. Ten replications of the outcome vector are obtained for each design. One of these replications is presented in Table A.1 of the Appendix. The procedure that was discussed in Section 2.2 is adopted and the estimates of $V_{.05}$ are obtained. The "true" response curve and the estimated response curve are plotted in Figures 5, 6, 7, and 8 for one replication, and presented in Table A.1. The estimates of $V_{.05}$ are obtained from these figures. For Design 1, the estimate of $V_{.05}$ is obtained as $\hat{V}^1_{.05} = 4$ from the estimated response curve in Figure 5. Similarly, the estimates of $V_{.05}$ for Designs 2, 3, and 4 are obtained as $\hat{V}^2_{.05} = 4$, $\hat{V}^3_{.05} = 10$, and $\hat{V}^4_{.05} = 16$.

For the sequential design, the response curve that is estimated in the first phase is presented in Figure 9 for the replication presented in Table A.1. The response curves estimated in phases 2 and 3 are plotted in Figures 10 and 11, respectively. The estimate of $V_{.05}$ is obtained from Figure 11 as $\hat{V}^5_{.05} = 8$.

Once the $\hat{V}^j_{.05}(\ell)$ values are obtained for $\ell = 1,\ldots,10$ for Design j , MSE^j can be computed as:

$$MSE^j = \frac{1}{10} \sum_{\ell=1}^{10} \left(\hat{V}^j_{.05}(\ell) - 22 \right)^2 .$$

MSE^j's for the Weibull response curve are presented in Table 1.

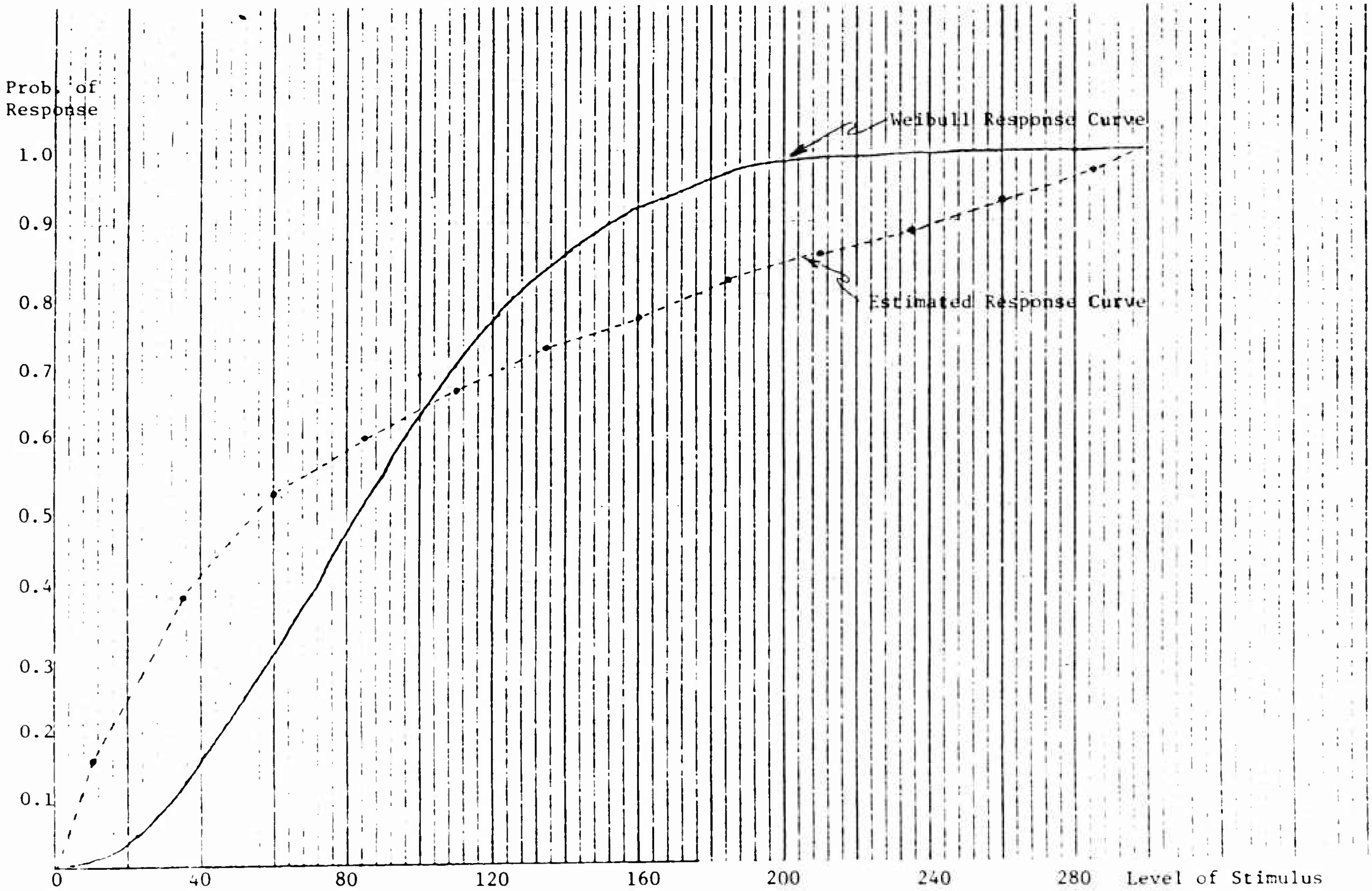

Figure 5. Design 1.

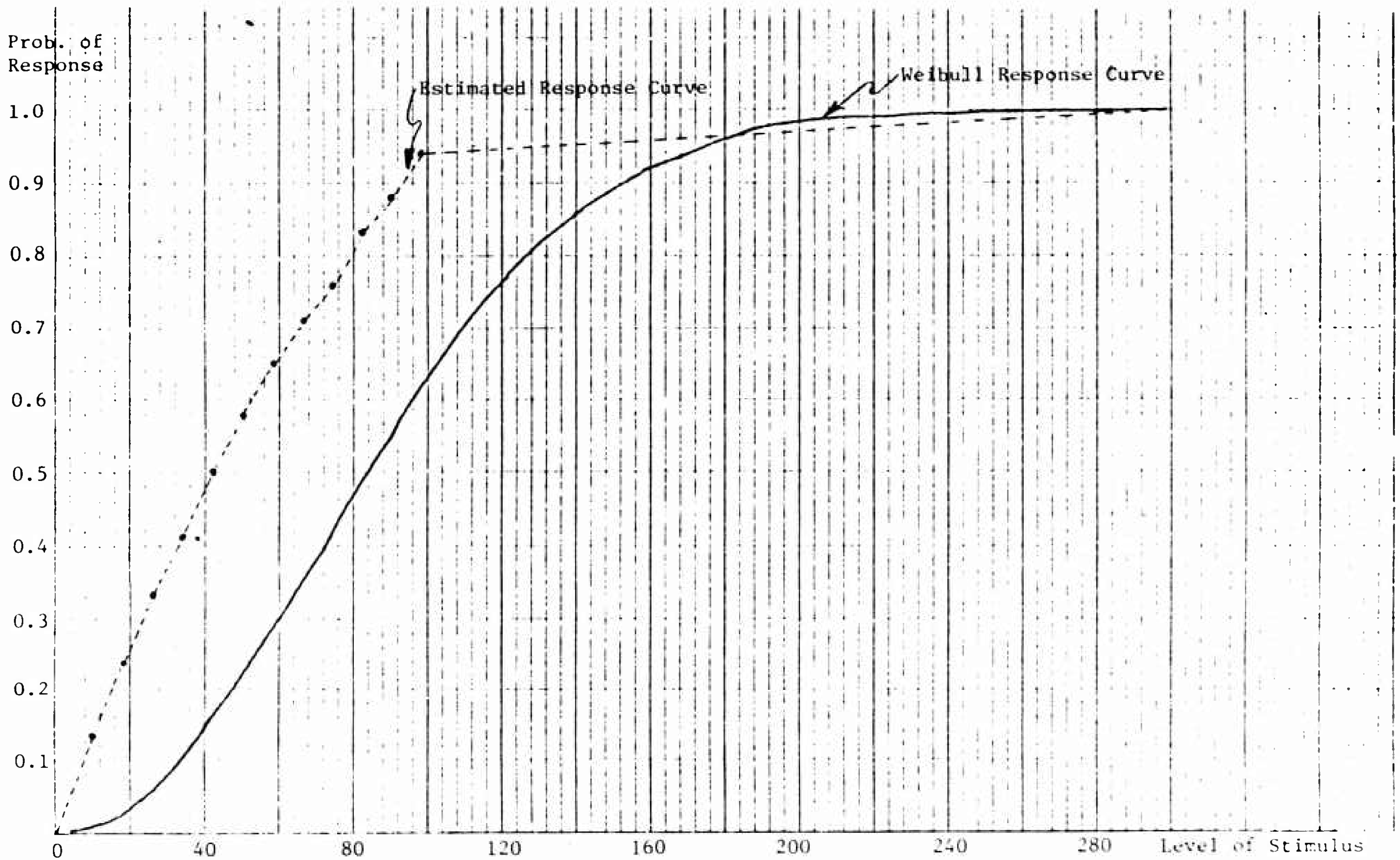

Figure 6. Design 2.

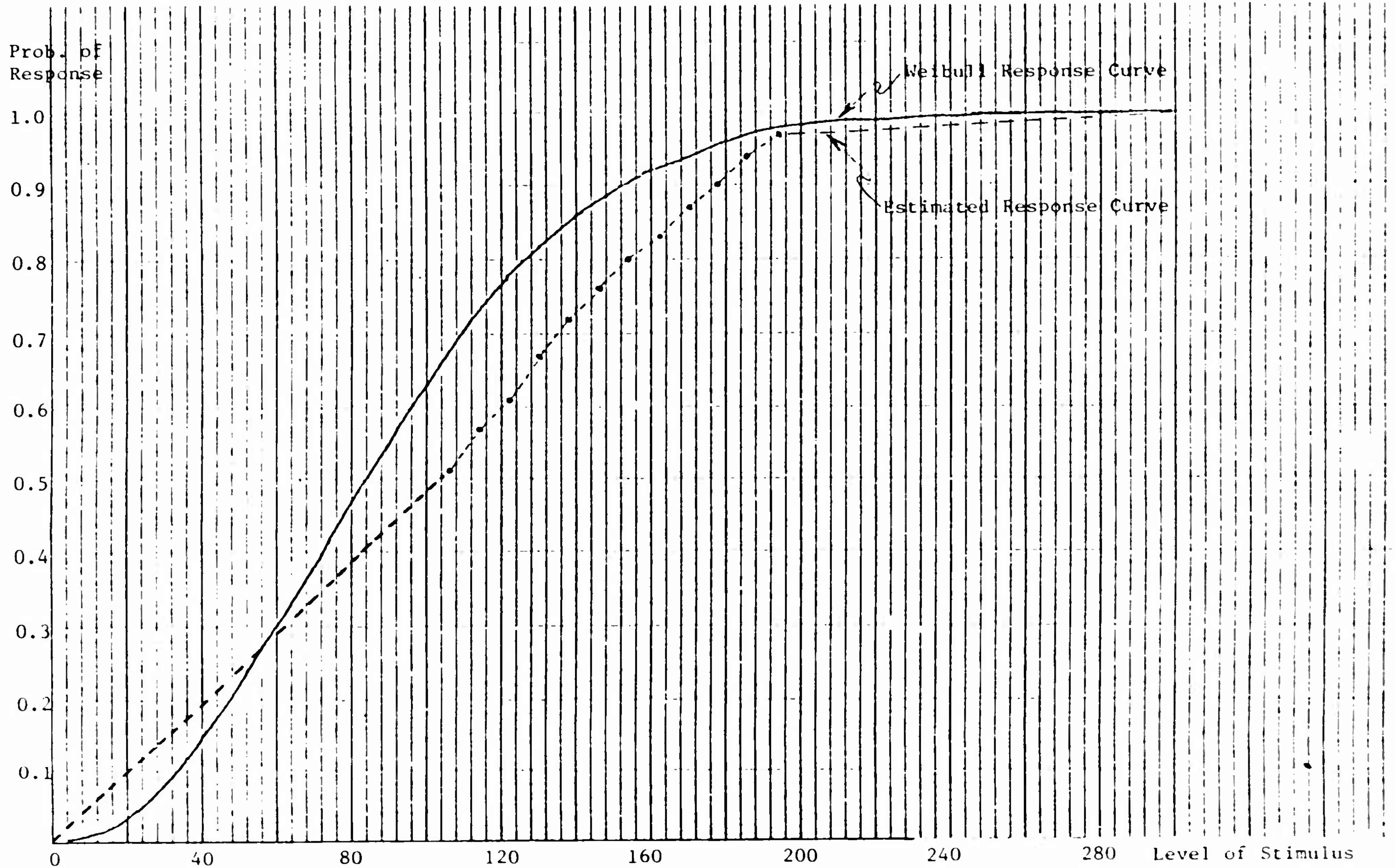

Figure 7. Design 3.

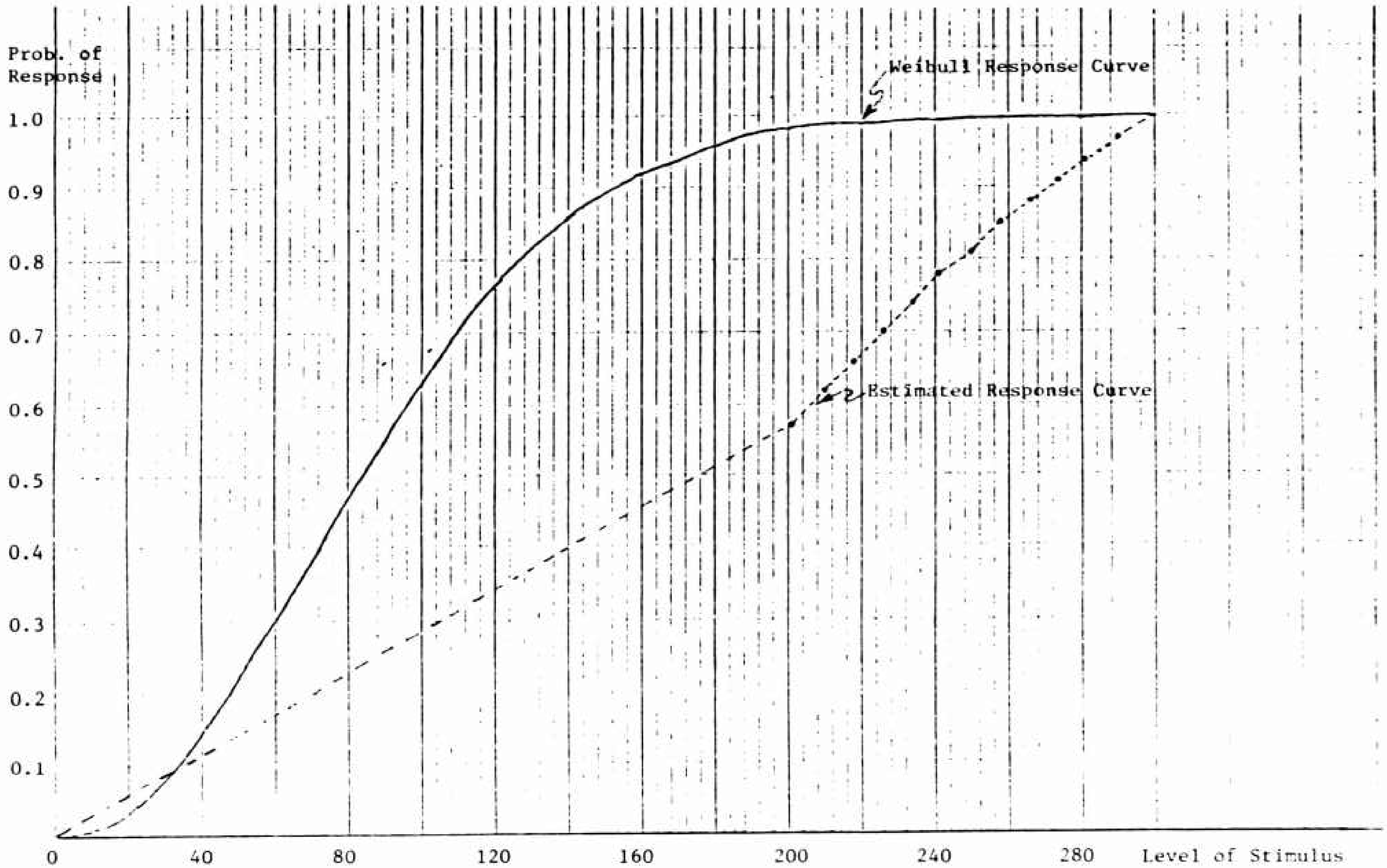

Figure 8. Design 4.

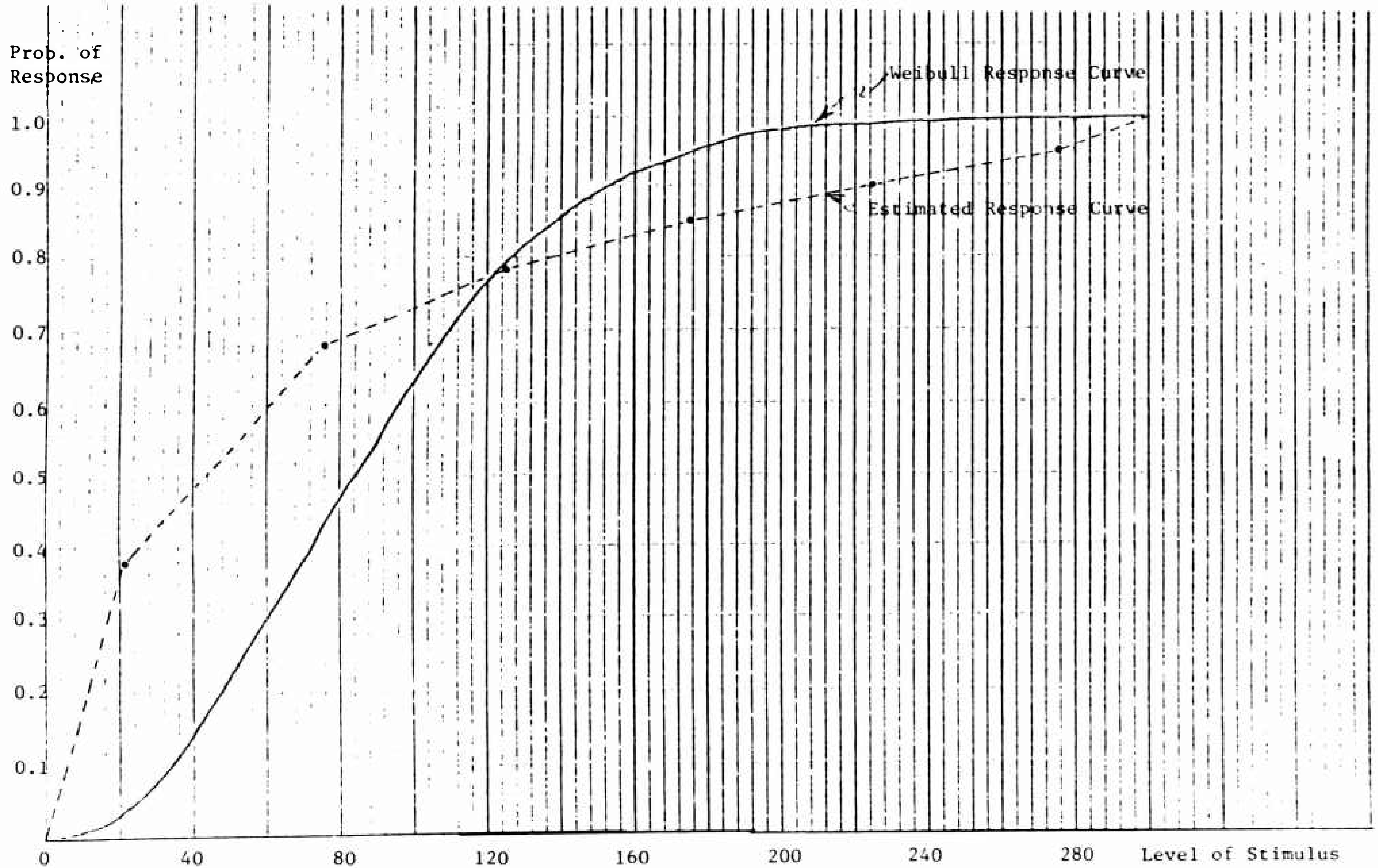

Figure 9. Sequential design, phase I.

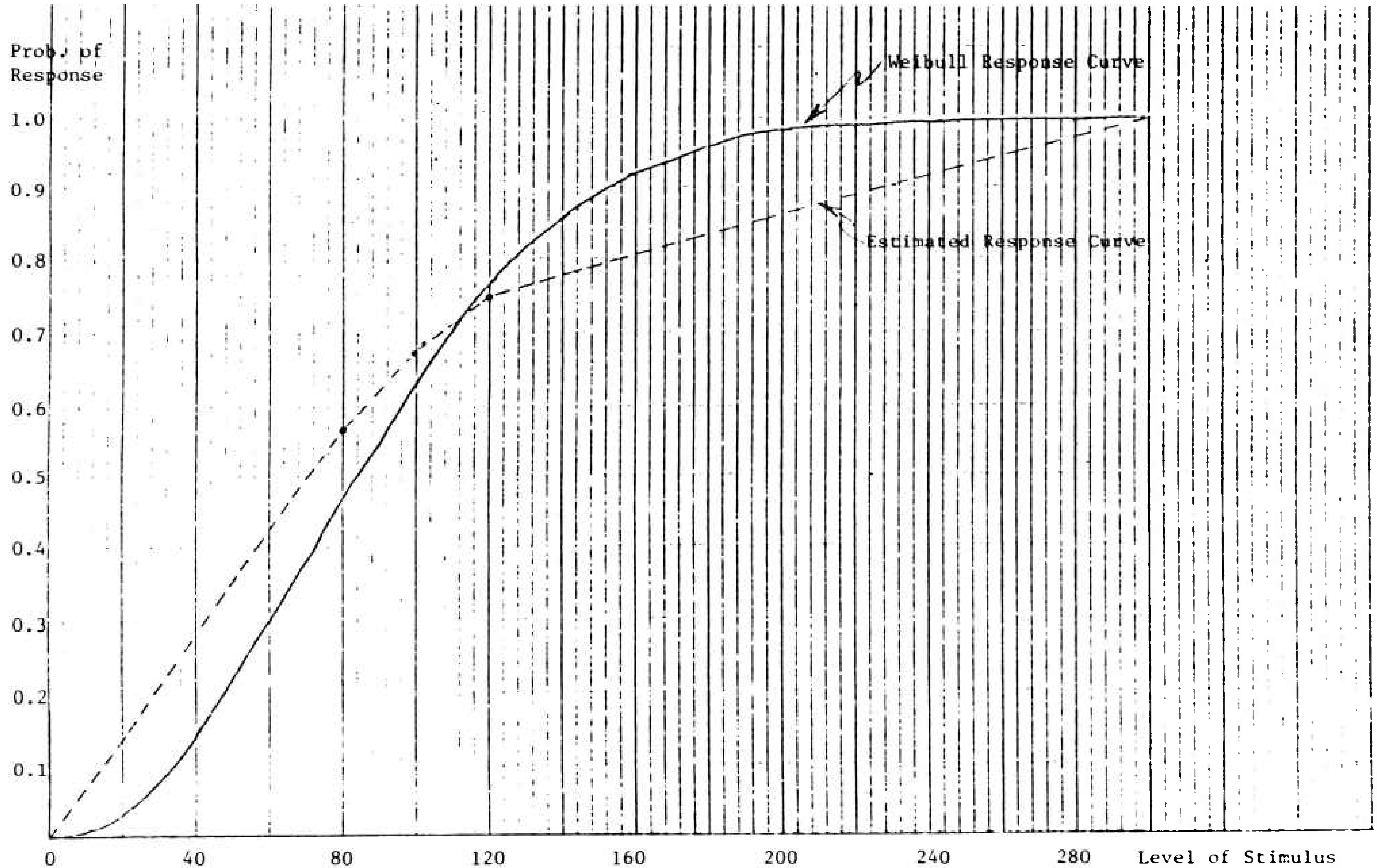

Figure 10. Sequential design, phase II.

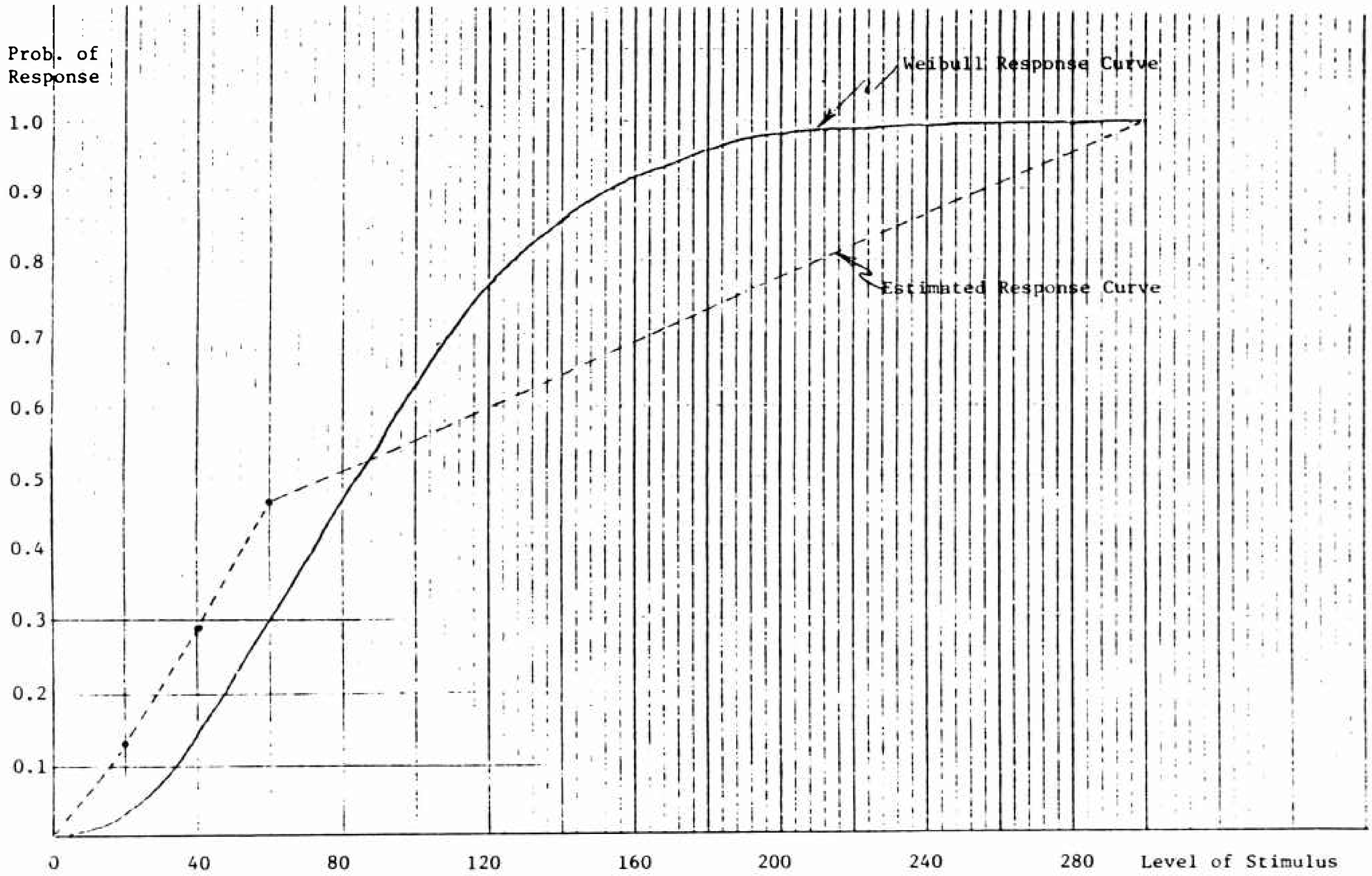

Figure 11. Sequential design, phase III.

Table 1. MSE's for the Weibull Response Curve

Design	MSE
1	360.1
2	320.2
3	126.2
4	36.0
5 (sequential)	196.8

The minimum MSE is obtained when Design 4 is selected; that is, when all k observations are concentrated in the right-hand half of the interval of the range of testing. The second lowest MSE is obtained when all k observations are concentrated in the center of the interval of the range of testing.

4.2 Analysis for the Lognormal Response Curve I

The second response curve is a lognormal distribution function where $V_{.05} = 52$. Again ten outcome vectors, $\underset{\sim}{X}^j$'s, are simulated for each design. The response curves are constructed and $\hat{V}^j$'s are obtained. The estimated response curves can be observed from Figures 12, 13, 14, and 15 for Designs 1, 2, 3, and 4, respectively, for a single replication. The estimates of $V_{.05}$ are $\hat{V}^1_{.05} = 4$, $\hat{V}^2_{.05} = 5$, $\hat{V}^3_{.05} = 11$, and $\hat{V}^4_{.05} = 18$ from the corresponding figures.

For the sequential design, Design 5, the response curves estimated in phases 1, 2, and 3 are plotted in Figures 16, 17, and 18, respectively. The estimate of $V_{.05}$ is obtained as $\hat{V}^5_{.05} = 9$ from Figure 18.

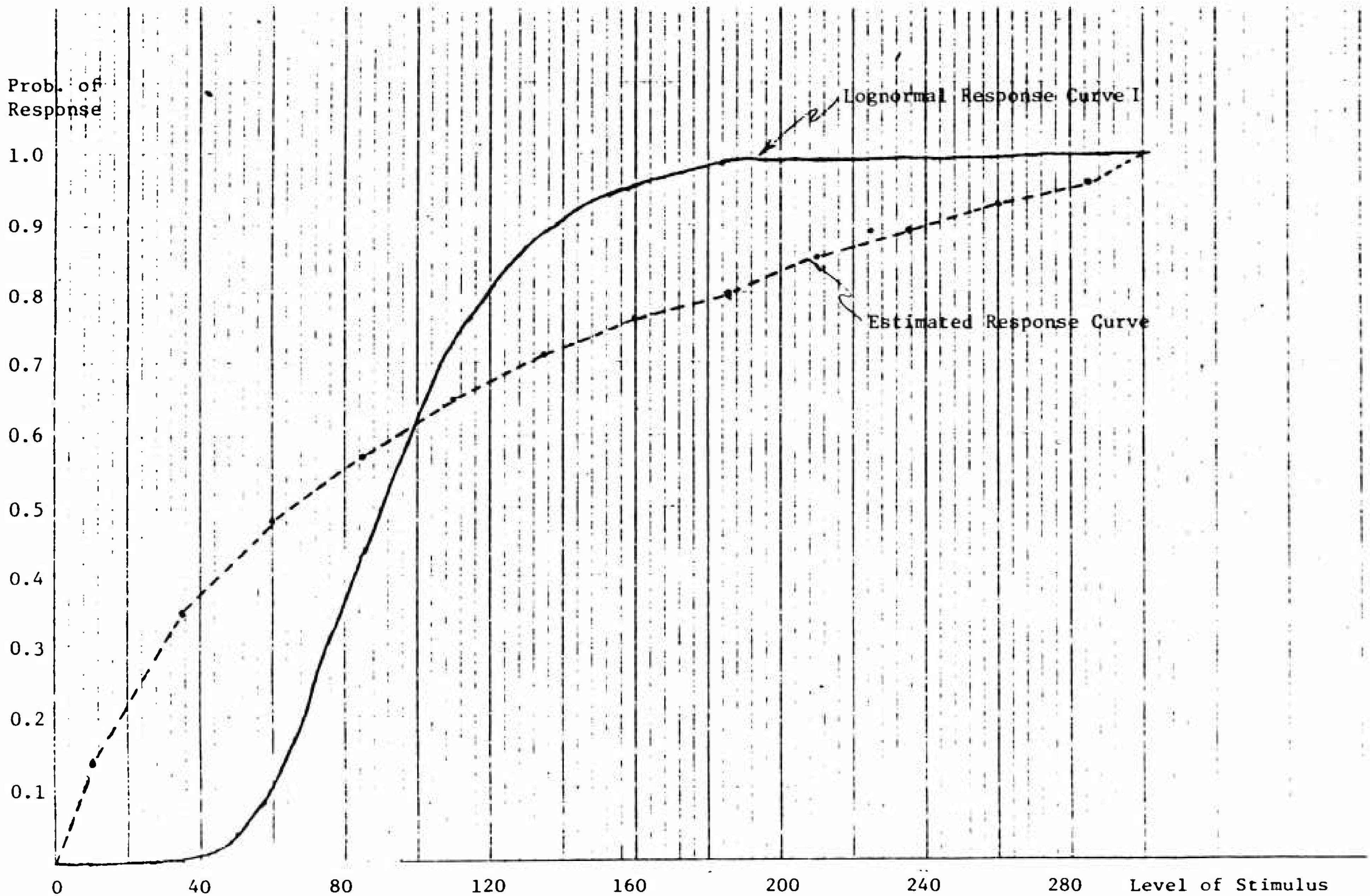

Figure 12. Design 1, lognormal.

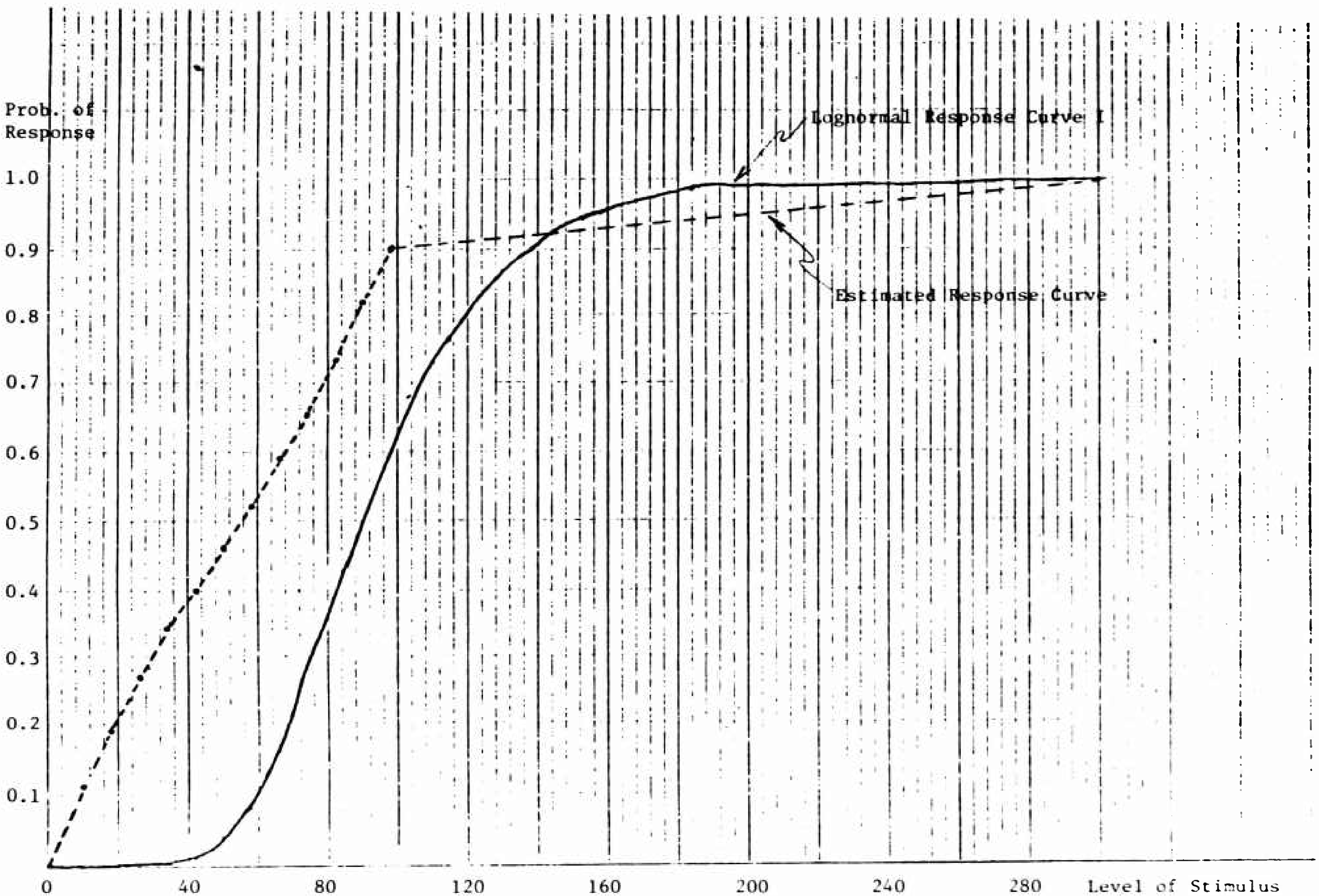

Figure 13. Design 2, lognormal.

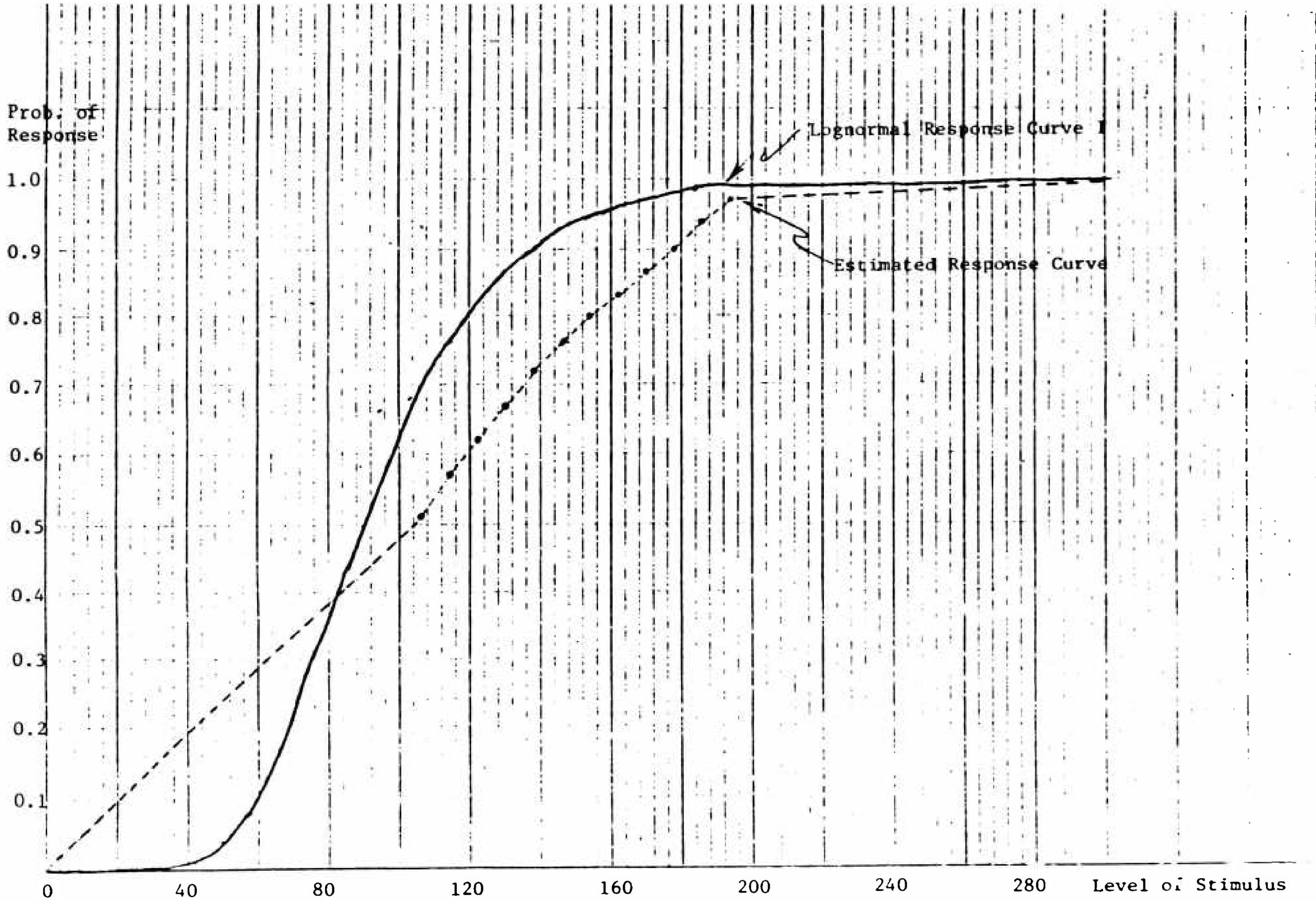

Figure 14. Design 3, lognormal.

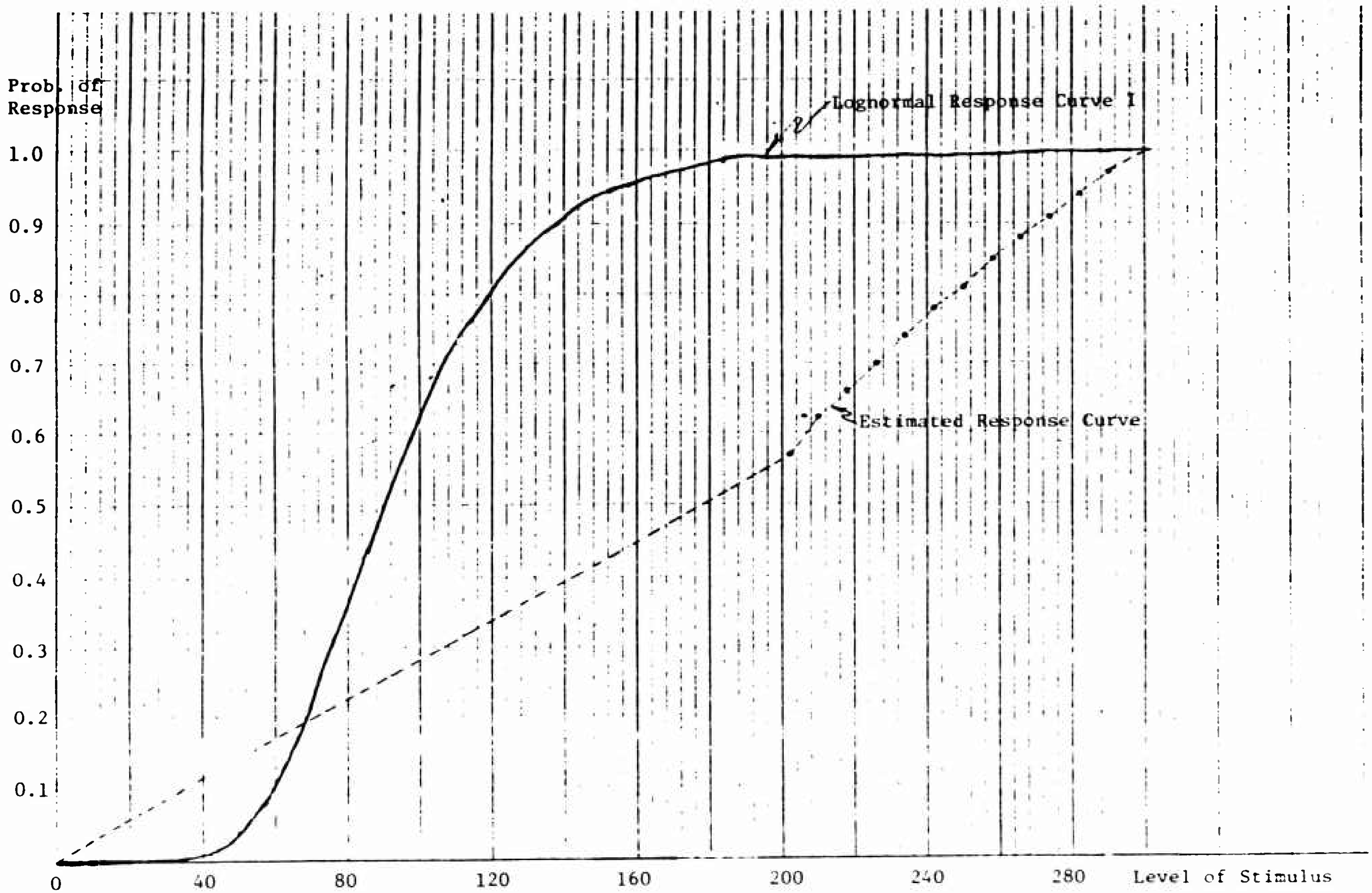

Figure 15. Design 4, lognormal.

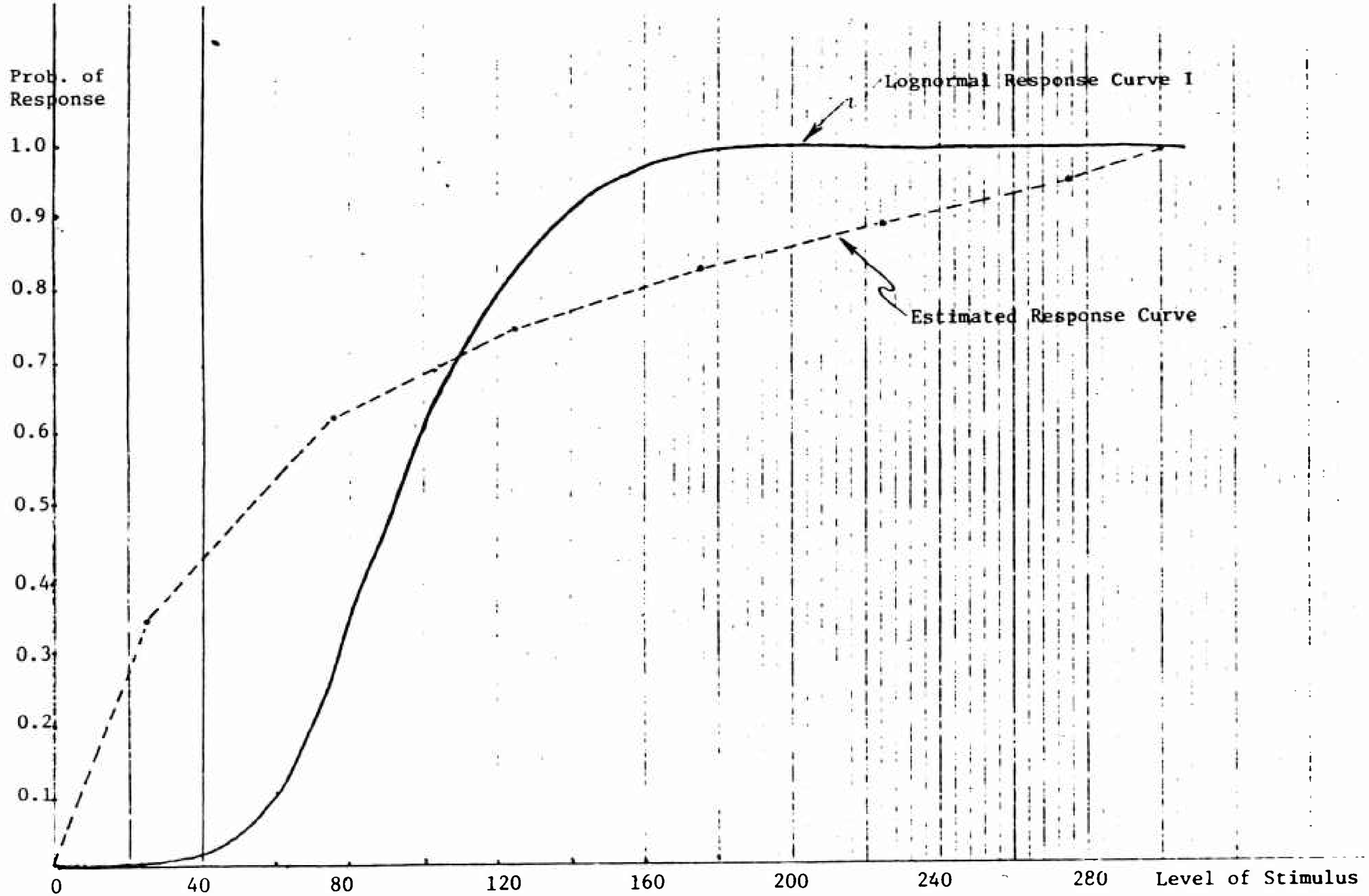

Figure 16. Sequential design, phase I, lognormal.

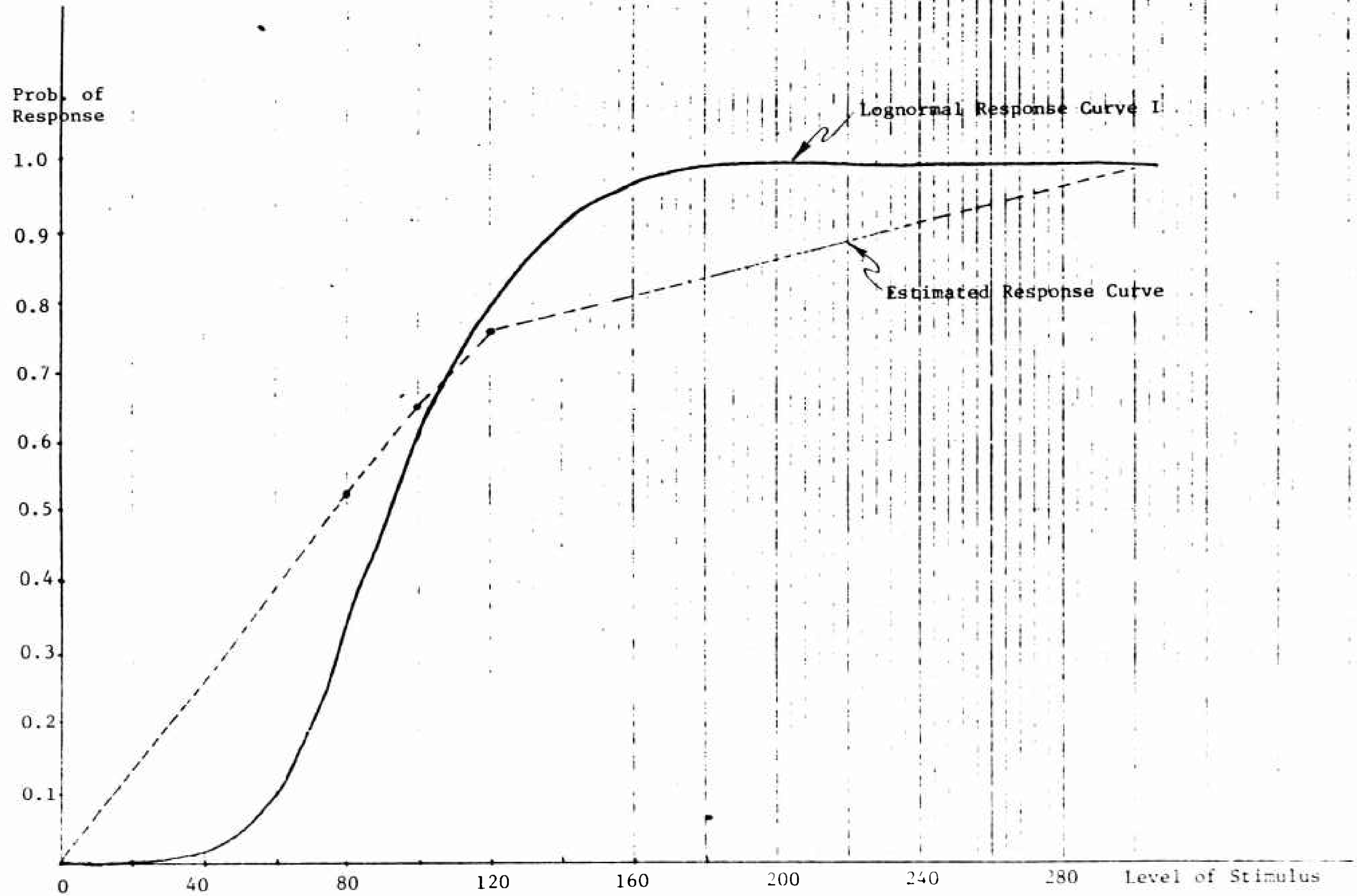

Figure 17. Sequential design, phase II, lognormal.

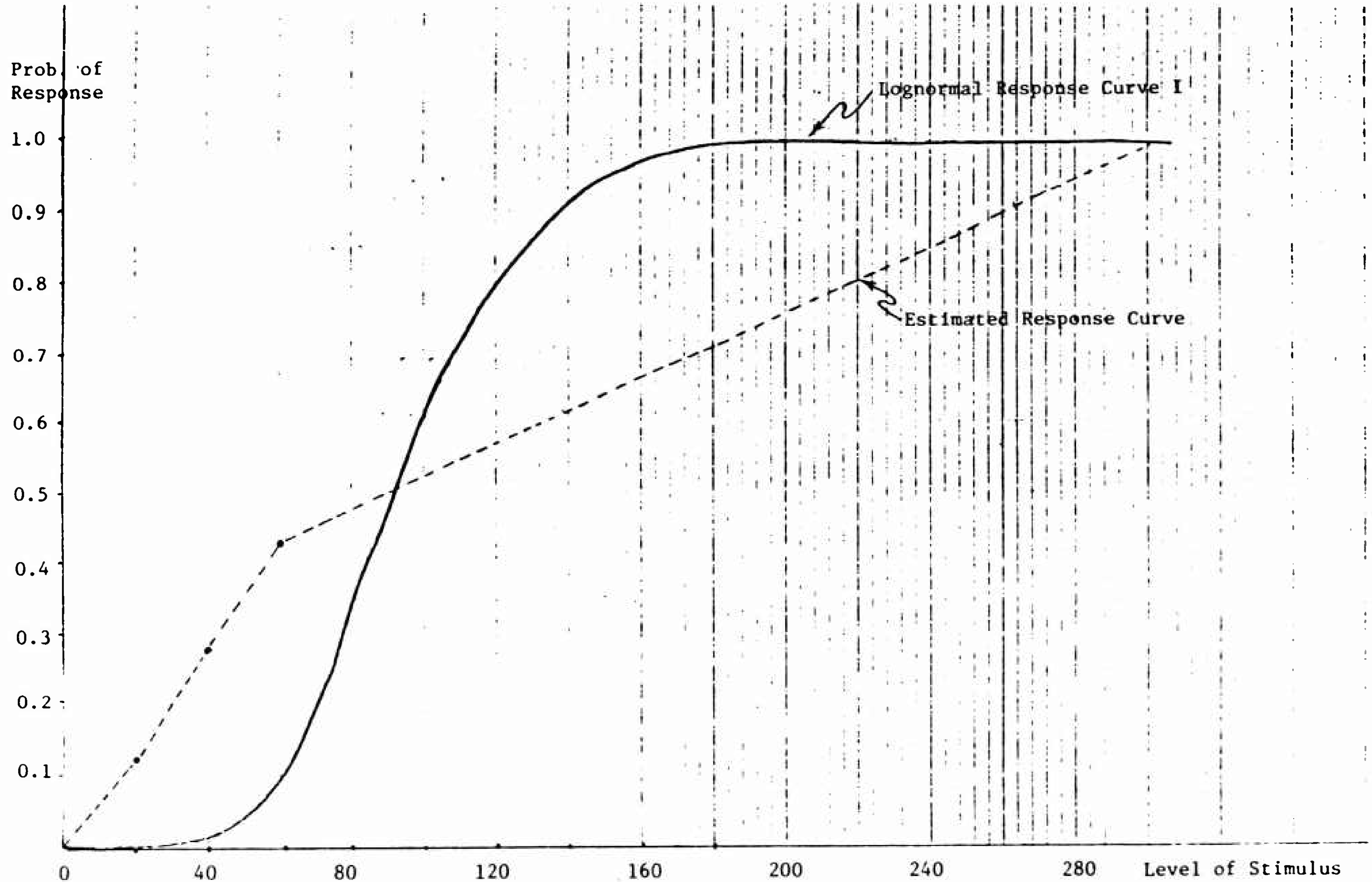

Figure 18. Sequential design, phase III, lognormal

Table 2. MSE's for the Lognormal Response Curve I

Design	MSE
1	2313.7
2	2209.0
3	1714.2
4	1142.8
5	1981.1

The MSE's computed for the lognormal response curve are presented in Table 2. As we can observe, the minimum MSE is obtained when Design 4 is selected. The second lowest MSE is obtained for Design 3.

4.3 Analysis for the Lognormal Response Curve II

The third response curve is also a lognormal distribution function, where $V_{.05} = 10$. The outcome vectors are simulated and the response curves are estimated as in the previous sections. The $\hat{V}^j_{.05}$ values are obtained using the estimated response curves for each design. The estimated response curves can be observed from Figures 19 – 22 for Designs 1, 2, 3, and 4 for a single replication. The estimates are obtained as $\hat{V}^1_{.05} = 2$, $\hat{V}^2_{.05} = 3$, $\hat{V}^3_{.05} = 10$, and $\hat{V}^4_{.05} = 19$.

For Design 5, the estimated response curves for phases 1 – 3 are presented in Figures 23 – 25. The estimate of $V_{.05}$ is obtained as $\hat{V}^5_{.05} = 3$ for the sequential design.

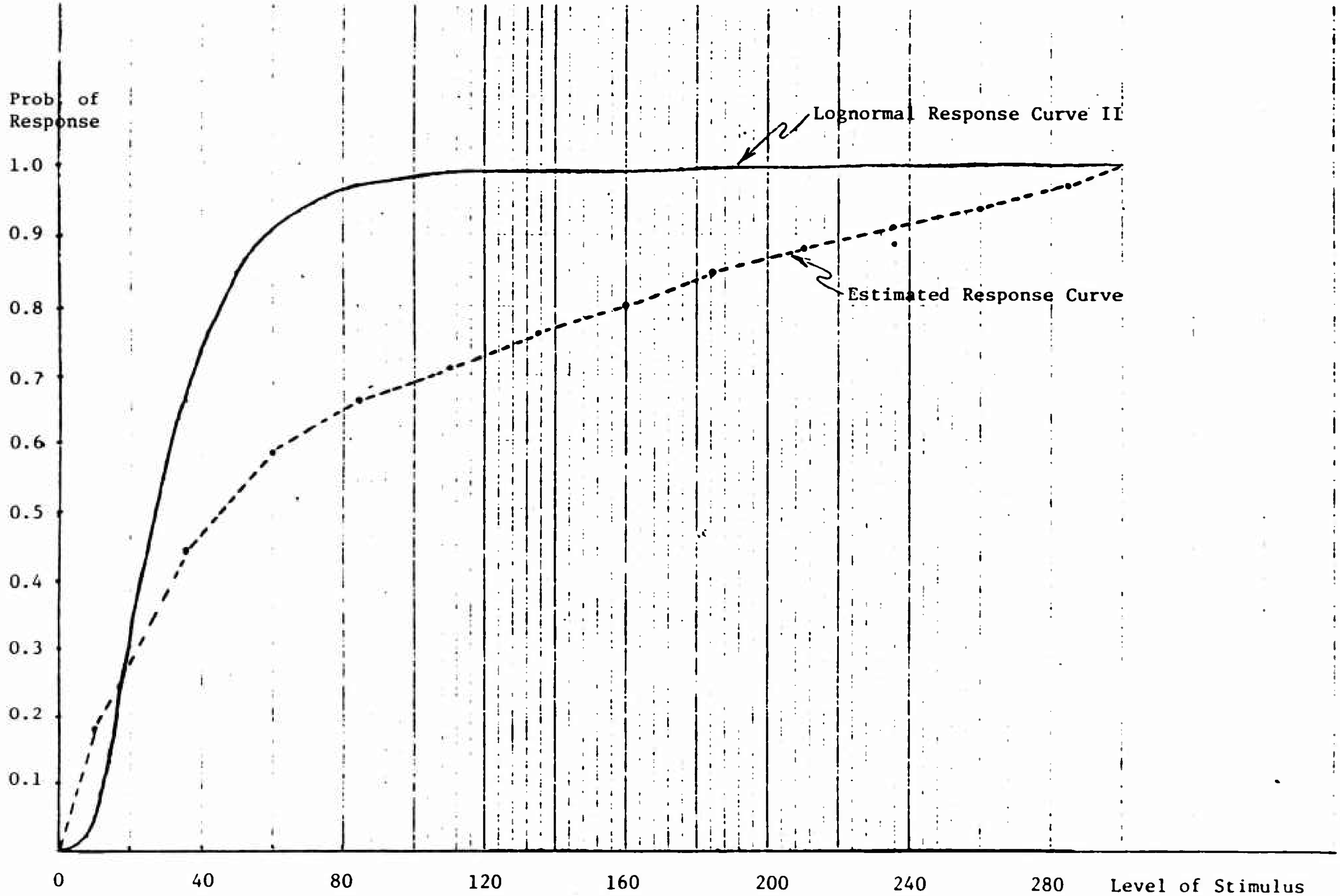

Figure 19. Design 1, lognormal II.

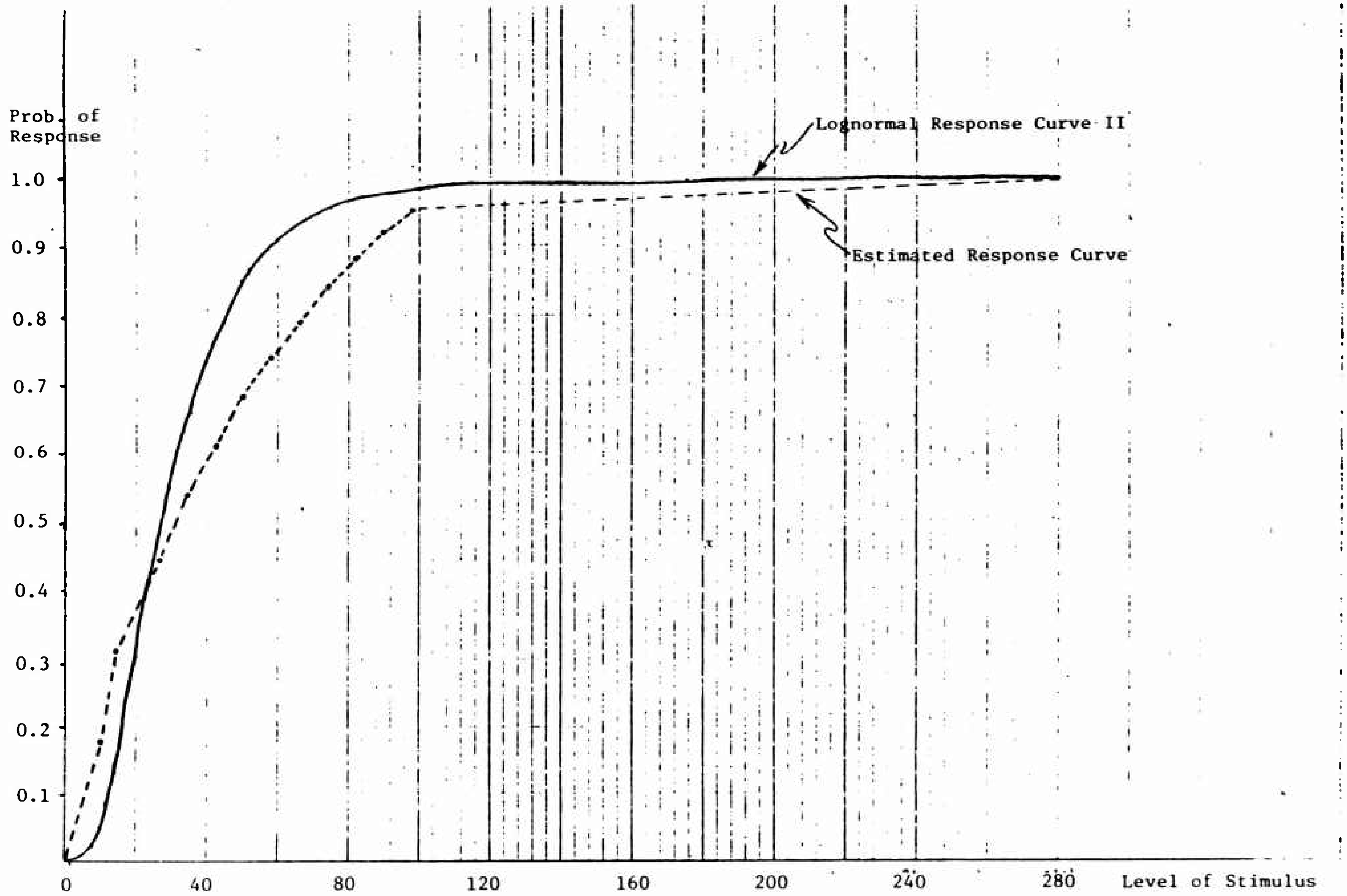

Figure 20. Design 2, lognormal II.

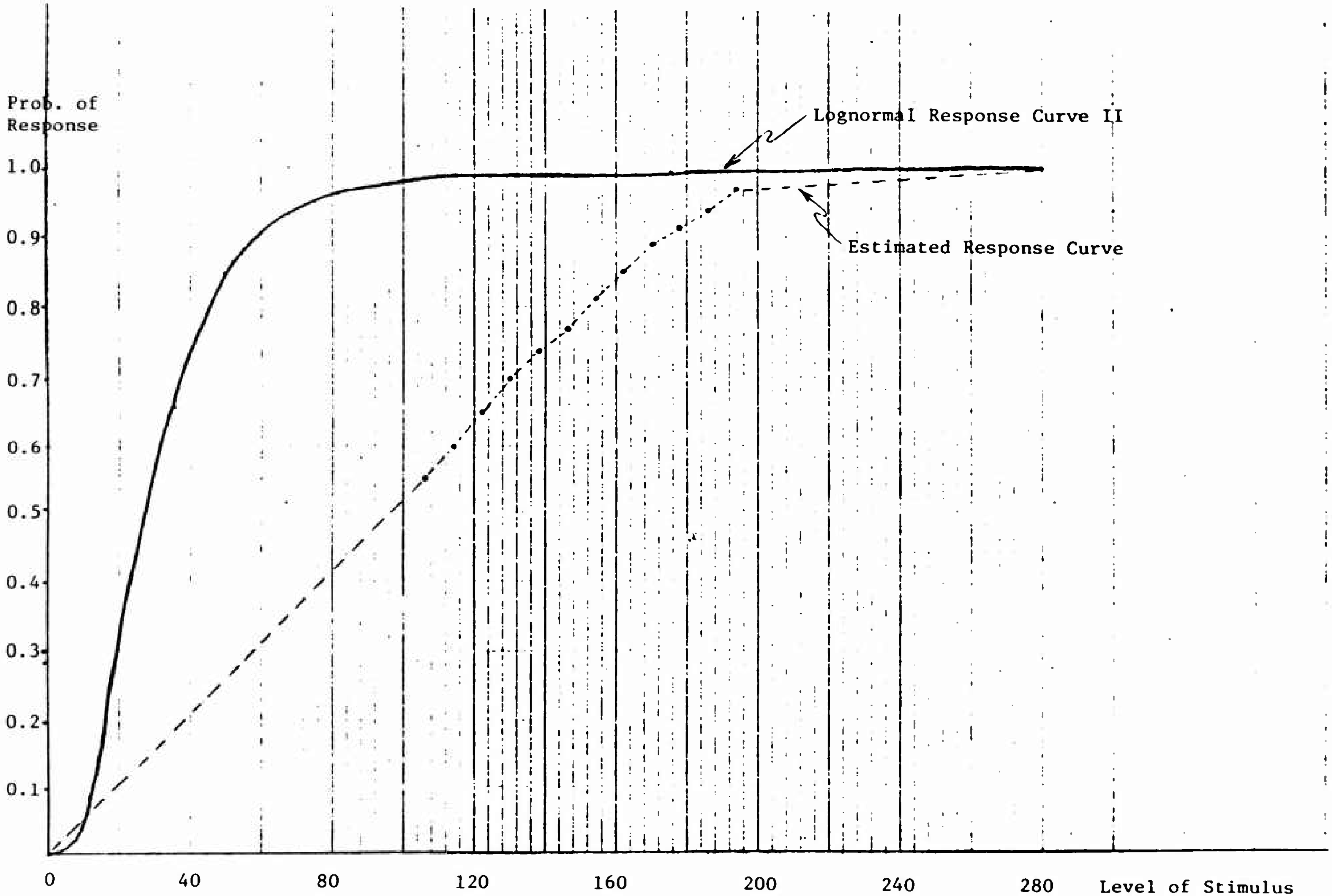

Figure 21. Design 3, lognormal II.

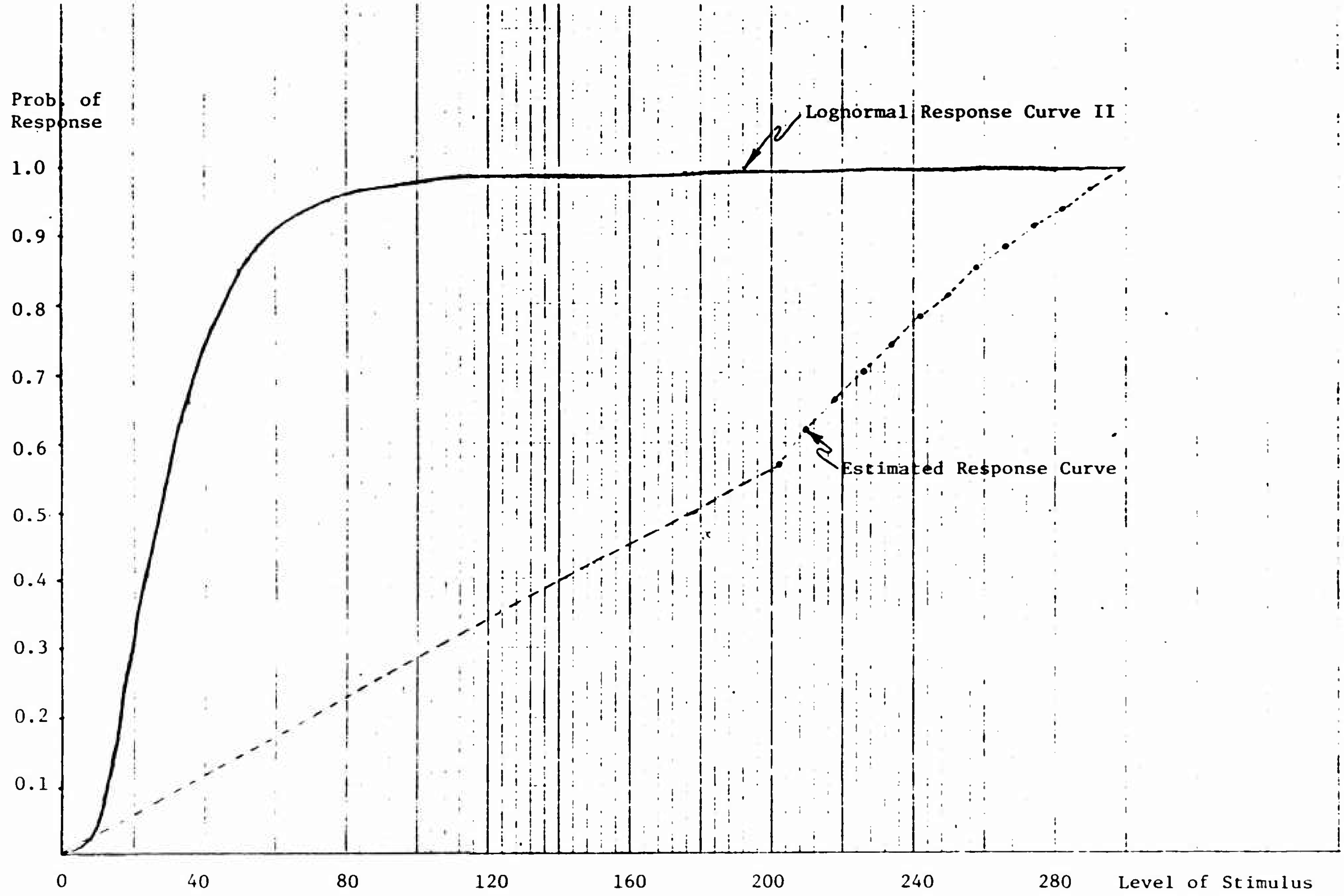

Figure 22. Design 4, lognormal II.

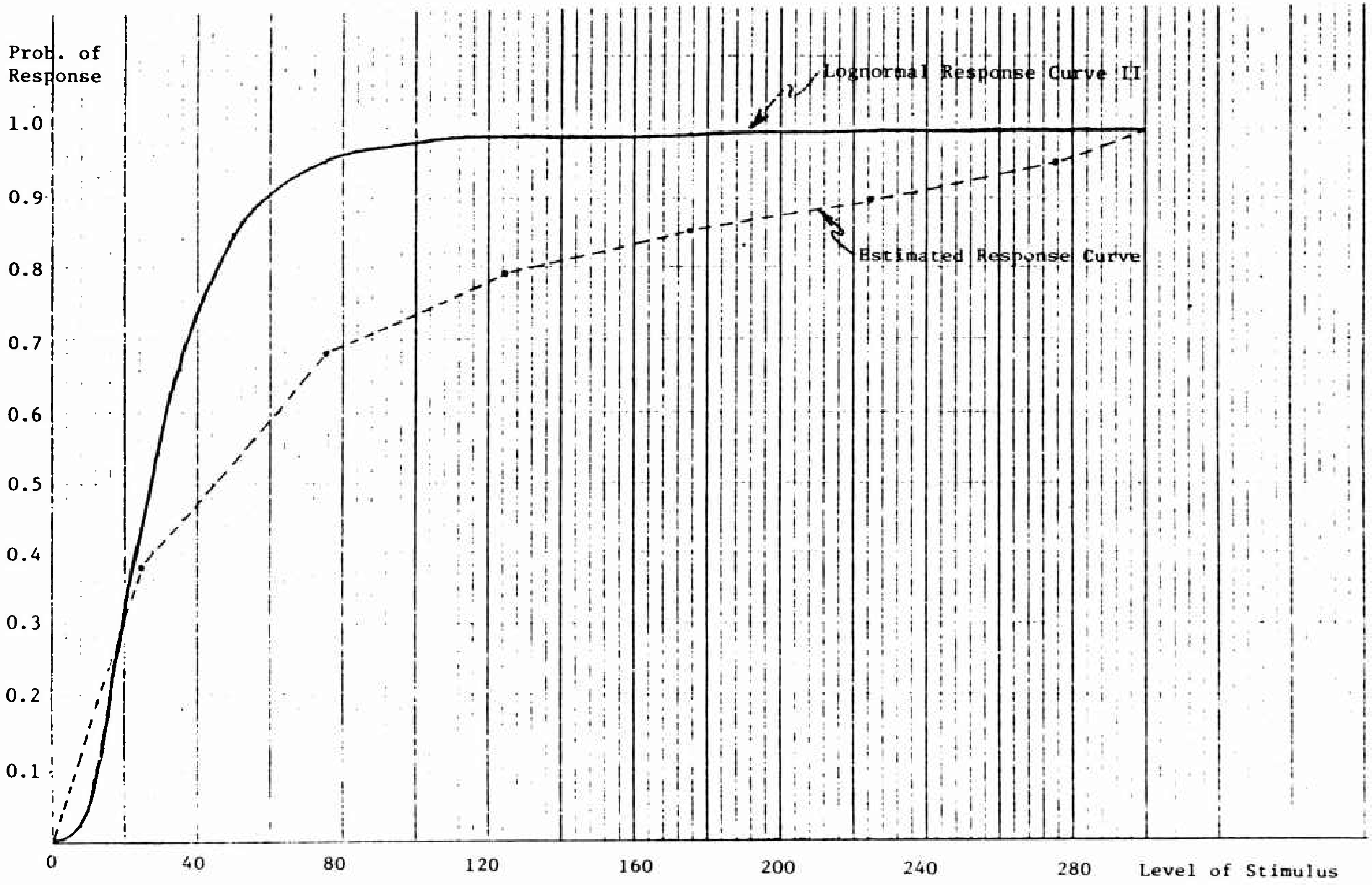

Figure 23. Sequential design, phase I, lognormal II.

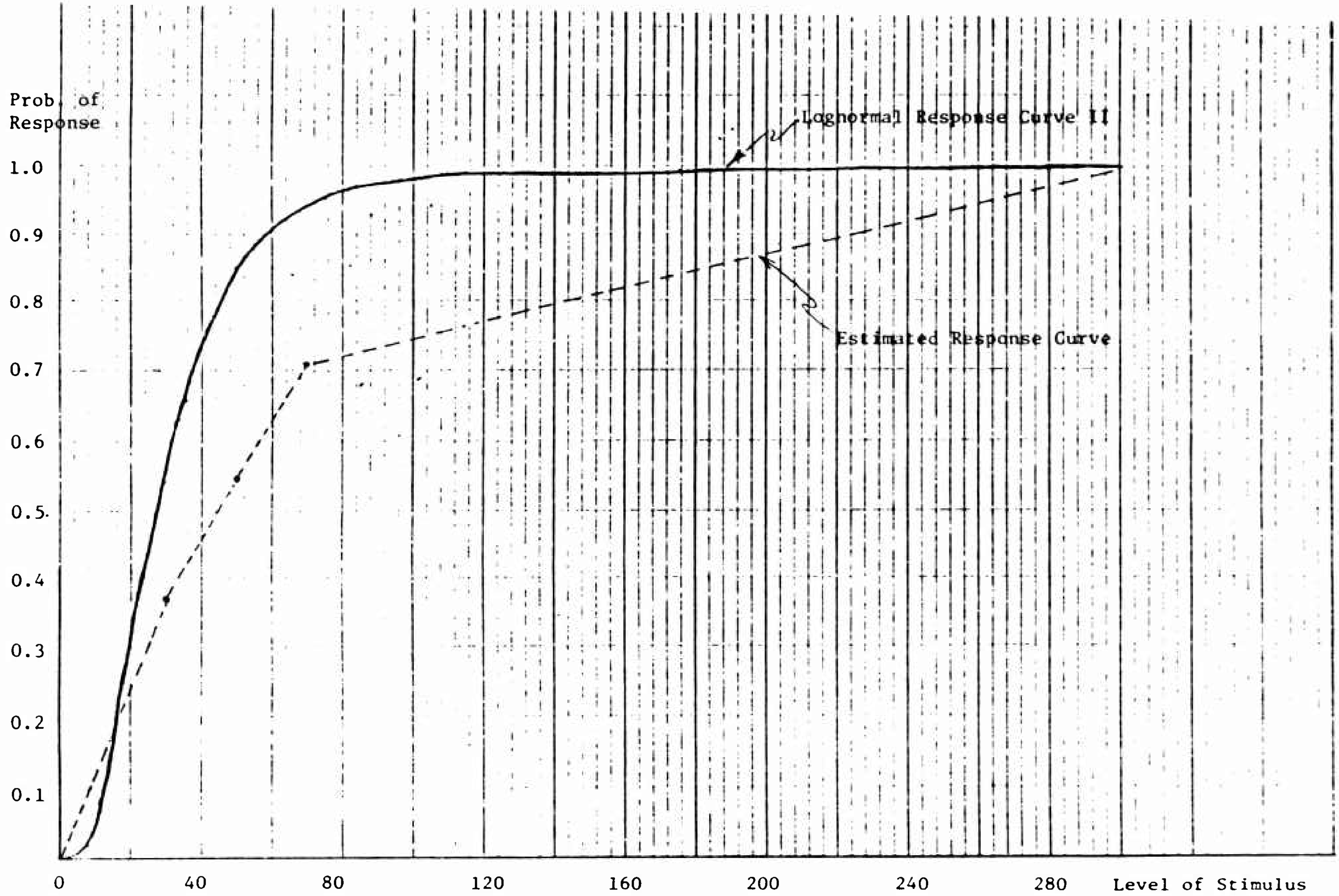

Figure 24. Sequential design, phase II, lognormal II.

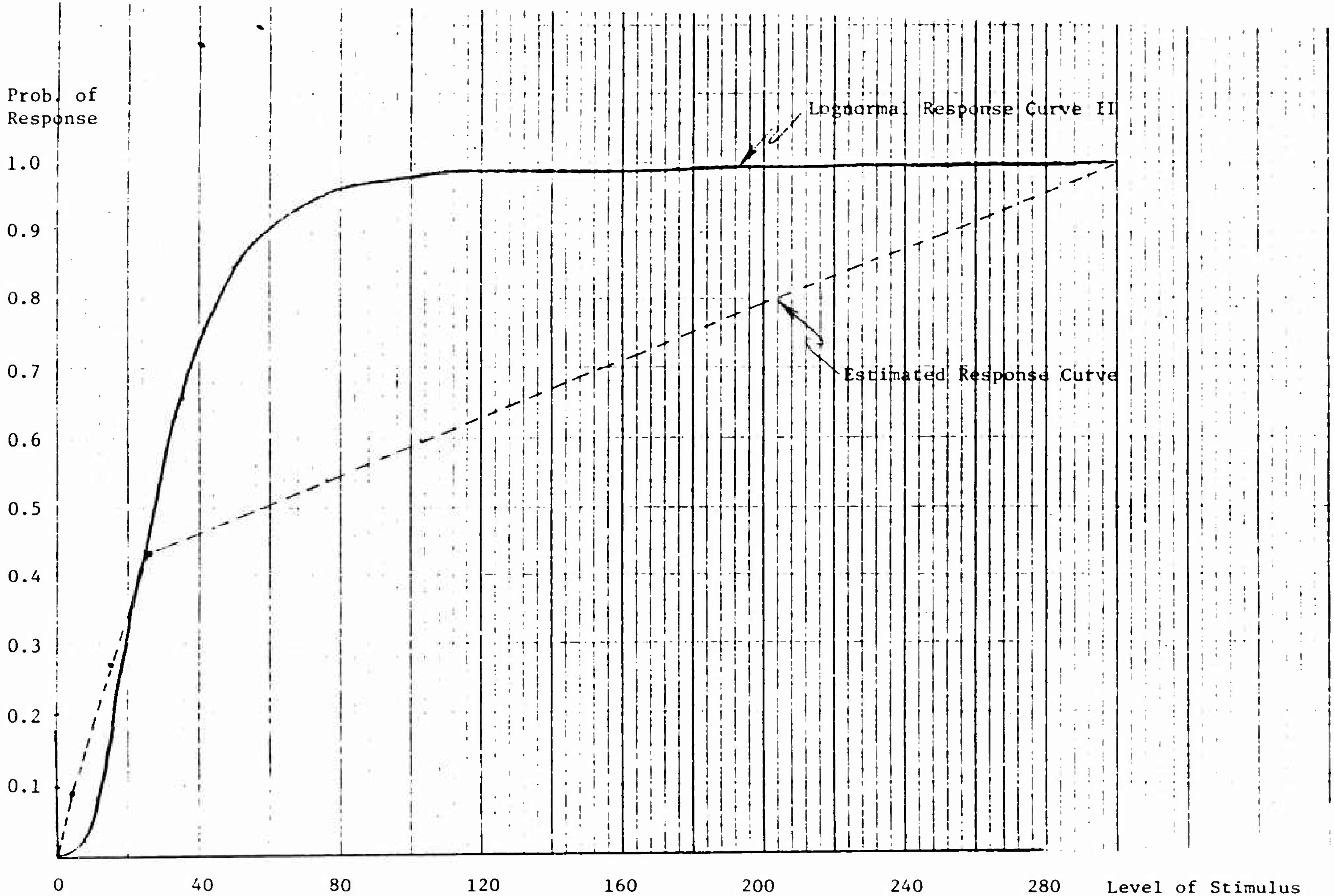

Figure 25. Sequential design, phase III, lognormal II.

Table 3. MSE's for the Lognormal Response Curve II

Design	MSE
1	53.7
2	55.0
3	0.4
4	144.0
5	46.8

The MSE's for the second lognormal response curve are presented in Table 3. We can observe from Table 3 that the minimum MSE is obtained for Design 3, where all 12 observations are concentrated in the center of the interval of the range of testing. The MSE obtained for Design 4 is the highest among them all. This indicates that the form of the "true" response curve affects the results significantly.

5. CONCLUSION

The application of our approach to simulated data from three types of response curve indicates that the shape of the "true" response curve is a significant factor in the evaluation of the estimate of $V_{.05}$. In real life, the "true" response curve is never known; therefore the experimenter should select his design based on his prior knowledge of the problem. Depending on the shape of the "true" response curve that is unknown to us, the $V_{.05}$ level might be underestimated or overestimated.

Sometimes the discrepancy is so large that one ends up with a high MSE for a given design, which is undesirable. The results obtained in Section 4 indicate that Design 2, where all k observations are concentrated in the left-hand half of the interval of the range of testing, has a tendency to underestimate $V_{.05}$ On the other hand, Design 4 has a tendency to overestimate $V_{.05}$ For the response curve that is considered in Section 4.3, this caused a high MSE for Design 4. The possibility of large discrepancies for these two designs makes them undesirable. The results of Section 4 also indicate that Design 3, where all k observations are concentrated in the center, gives better estimates of $V_{.05}$ in general. The discrepancies due to overestimation or underestimation are not large. This makes Design 3 more desirable than the others.

However, one should note that there is the difficulty of determining the region where the k observations will be concentrated. If the experiment has to be performed in a single phase, this region can be determined by using past information available to the investigator. Another possibility is to choose the middle portion of the interval of the range of testing.

On the basis of the analysis made, we can conclude that a design where the observations are concentrated in a region that provides the experimenter with more information is suitable for this problem. Therefore, in our analysis Design 3 is suggested as a suitable design for the estimation of $V_{.05}$. However, one should recall that the selection of the design must always be made on the basis of prior information that is available to the experimenter.

ACKNOWLEDGMENT. The work that is reported here was performed under the direction of Professer Nozer Singpurwalla. His helpful comments and advise in the preparation of the report are acknowledged.

APPENDIX

TABLES

Table A1. Data Simulated from the Weibull Response Curve

Design 1		Design 2		Design 3		Design 4		Sequential Design	
Level of Stimulus	Response	Level of Stimulus	Response	Level of Stimulus	Response	Level of Stimulus	Response	Level of Stimulus	Response
10	0	10	0	106	0	202	1	*Phase I:*	
35	0	18	0	114	1	210	1	25	0
60	1	26	0	122	0	218	1	75	1
85	0	34	0	130	1	226	1	125	1
110	1	42	0	138	1	234	1	175	1
135	1	50	1	146	1	242	1	225	1
160	1	58	1	154	1	250	1	275	1
185	1	66	1	162	1	258	1	*Phase II:*	
210	1	74	0	170	1	266	1	80	1
235	1	82	1	178	1	274	1	100	1
260	1	90	1	186	1	282	1	120	0
285	1	98	1	194	1	290	1	*Phase III:*	
								20	0
								40	0
								60	0

Table A2. Data Simulated from the Lognormal Response Curve I

Design 1		Design 2		Design 3		Design 4		Sequential Design	
Level of Stimulus	Response	Level of Stimulus	Response	Level of Stimulus	Response	Level of Stimulus	Response	Level of Stimulus	Response
10	0	10	0	106	0	202	1	*Phase I:*	
35	0	18	0	114	1	210	1	25	0
60	0	26	0	122	1	218	1	75	0
85	0	34	0	130	1	226	1	125	1
110	1	42	0	138	1	234	1	175	1
135	1	50	0	146	1	242	1	225	1
160	1	58	0	154	1	250	1	275	1
185	1	66	0	162	1	258	1	*Phase II:*	
210	1	74	0	170	1	266	1	80	0
235	1	82	0	178	1	274	1	100	1
260	1	90	1	186	1	282	1	120	1
285	1	98	1	194	1	290	1	*Phase III:*	
								20	0
								40	0
								60	0

Table A3. Data Simulated from the Lognormal Response Curve II

Design 1		Design 2		Design 3		Design 4		Sequential Design	
Level of Stimulus	Response	Level of Stimulus	Response	Level of Stimulus	Response	Level of Stimulus	Response	Level of Stimulus	Response
10	0	10	0	106	1	202	1	*Phase I:*	
35	1	18	0	114	1	210	1	25	0
60	1	26	1	122	1	218	1	75	1
85	1	34	1	130	1	226	1	125	1
110	1	42	1	138	1	234	1	175	1
135	1	50	1	146	1	242	1	225	1
160	1	58	1	154	1	250	1	275	1
185	1	66	1	162	1	258	1	*Phase II:*	
210	1	74	1	170	1	266	1	30	0
235	1	82	1	178	1	274	1	50	1
260	1	90	1	186	1	282	1	70	1
285	1	98	1	194	1	290	1	*Phase III:*	
								5	0
								15	0
								25	1

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